JESS

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JESS is a package intended as a research tool for performing chemical calculations in aqueous solution and associated other phases. It has a substantial database of thermodynamic parameters for supporting chemical equilibrium calculations (over 208,000 constants for some 70,000 chemical reactions). The equilibrium calculations can be coupled with kinetic processes. The package has been used extensively for modelling large chemical systems of environmental, biological and industrial interest. Its special focus is to help understand, and to help remedy, the errors which frequently afflict chemical speciation models published in the literature.